

# Old Dominion University Research Foundation

DEPARTMENT OF MATHEMATICAL SCIENCES  
COLLEGE OF SCIENCES  
OLD DOMINION UNIVERSITY  
NORFOLK, VIRGINIA 23529

Langley  
GRANT  
111-36-CR  
253020  
47 p.

## THEORETICAL STUDIES OF SOLAR LASERS AND CONVERTERS

By

John H. Heinbockel, Principal Investigator

Progress Report  
For the period May 15, 1989 to December 31, 1989

Prepared for  
National Aeronautics and Space Administration  
Langley Research Center  
Hampton, Virginia 23665

Under  
Research Contract NAG-1-757  
Dr. Robert C. Costen, Technical Monitor  
SSD-High Energy Science Branch

January 1990

(NASA-CR-106194) THEORETICAL STUDIES OF  
SOLAR LASERS AND CONVERTERS Progress Report,  
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CSCL 20F

N90-14583

Unclas  
G3/36 0253020

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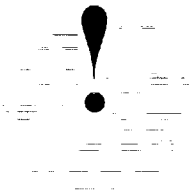
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Submitted by the  
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P.O. Box 6369  
Norfolk, Virginia 23508-0369

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# THEORETICAL STUDIES OF SOLAR LASERS AND CONVERTERS

By

John H. Heinbockel\*

Research for the period consisted of developing and refining the continuous flow laser model program. In addition, a working model for a two pass continuous wave amplifier was developed. The following is a summary of the mathematical development of a two pass amplifier for the  $n\text{-C}_3\text{F}_7\text{I}$  iodine laser. The geometry of the amplifier is illustrated in Figure 1. In this figure

- $P_{in}$  - power density into the amplifier ( $\text{watts/cm}^2$ ),
- $W$  - transmission coefficient,
- $\epsilon$  - radiation energy from  $I^*$  ( $\text{watt-sec}$ ),
- $C$  - speed of light,
- $P_{out}$  - output power density,
- $R_L$  - reflection coefficient for mirror,
- $\rho_+(Z)$  - photon density for wave motion in positive direction ( $\text{cm}^{-3}$ ),
- $\rho_-(Z)$  - photon density for wave motion in negative direction ( $\text{cm}^{-3}$ ).

The input power density  $P_{in}$  is assumed to be known. The photon density satisfies for all values  $Z$

$$\rho_+(Z) - \rho_-(Z) = K_0 \tag{1}$$

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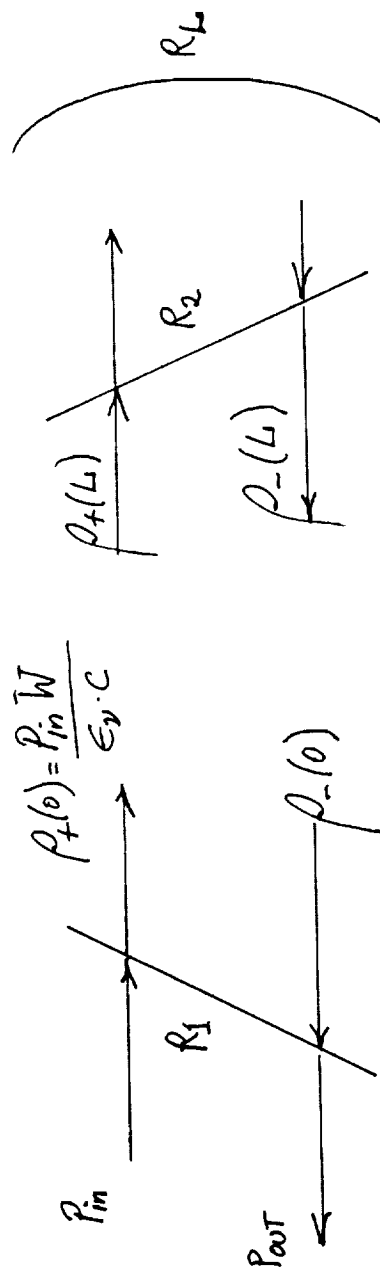


Figure 1. Geometry for Two Pass Amplifier.

where  $K_0$  is a constant. At  $Z = 0$  we have

$$\rho_+(0)\rho_-(0) = K_0 \quad (2)$$

and at  $Z = L$  we have

$$\rho_+(L)\rho_-(L) = K_0. \quad (3)$$

The value of  $\rho_+(0)$  is determined from the assumed value for the input power density  $P_{in}$  and from this we calculate

$$\rho_+(0) = \frac{P_{in} W}{\epsilon C} \quad (4)$$

and consequently from the relation (2) we have

$$\rho_-(0) = \frac{K_0}{\rho_+(0)}.$$

In the above relations  $W$  is the transmission coefficient of the Brewster windows and  $K_0$  is an assumed initial value. At  $Z = L$  we have  $R_2 = W^2 R_L$  as the reflection coefficient from the Brewster window. We then are able to calculate the return photon density from the Brewster window at  $Z = L$ . We find that this density should have the value

$$\rho_-(L) = R_2 \rho_+(L). \quad (5)$$

Combining the equations (2) (3) and (5) we determine that

$$R_2 \rho_+^2(L) = K_0 \quad \text{or} \quad \rho_+(L) = \sqrt{\frac{K_0}{R_2}} = \sqrt{\frac{\rho_+(0) \rho_-(0)}{R_2}} \quad (6)$$

Using the value (6) as the theoretical value for  $\rho_+(L)$  at  $Z = L$  we can compare this value with the calculate value for  $\rho_+(L)$  obtained from an integration of the differential equations defining the chemical reactions occurring in the amplifier. We adjust the value for  $\rho_-(0)$  until

$$\left| \rho_+(L)_{\text{theoretical}} - \rho_+(L)_{\text{calculated}} \right| < E \quad (7)$$

where  $E$  is an error criteria.

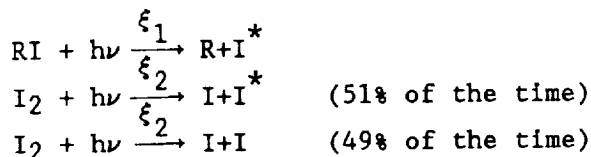
The above procedure is a shooting method for the determination of  $\rho_-(0)$ . When the error criteria is satisfied, the output power is obtainable from the relation

$$P_{\text{out}} = \rho_-(0) W \varepsilon C \quad (8)$$

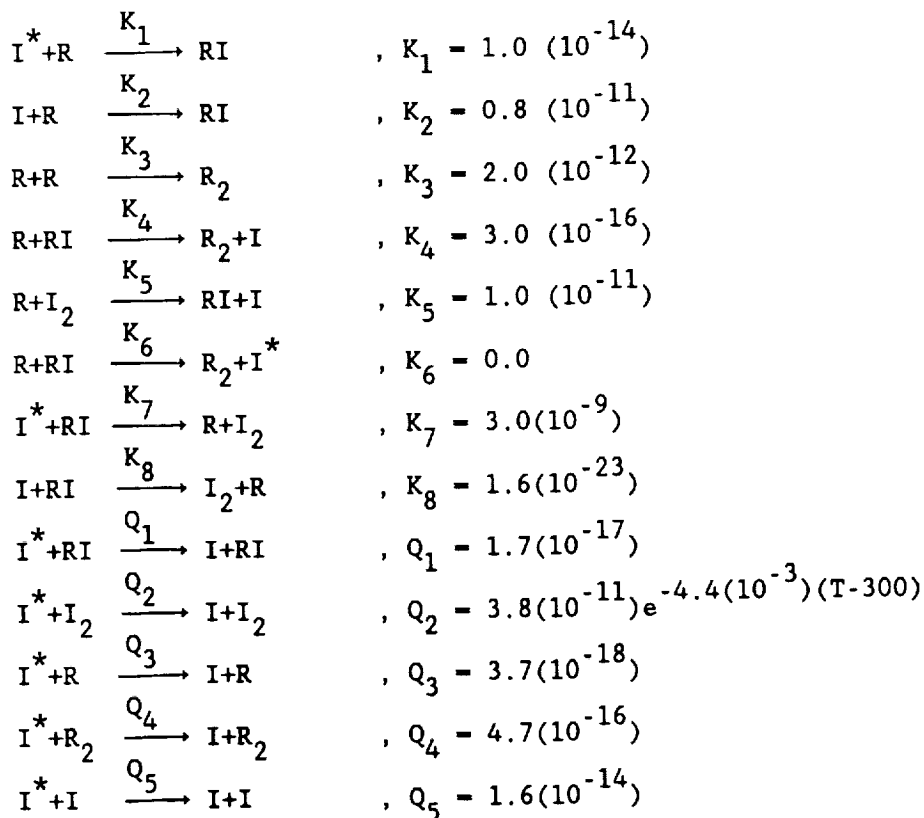
and the gain is calculated from the relation

$$\text{gain} = 10 \log_{10} \left( \frac{P_{\text{out}}}{P_{\text{in}}} \right) \text{ (decibels)}. \quad (9)$$

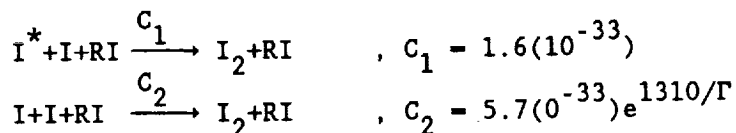
The chemical reactions occurring in the laser tube are listed along with the values used for the rate constant. The assumed reactions are:

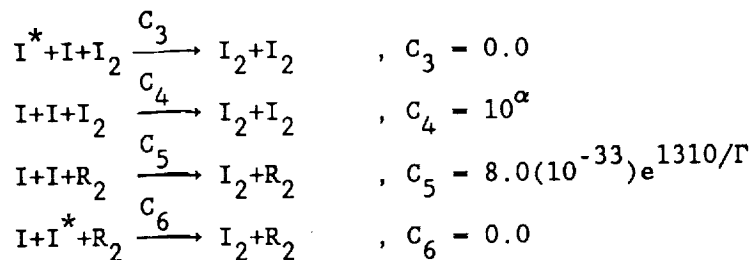


### Two Body Reactions



### Three Body Reactions





where

$$\alpha = -29.439 - 5.844 \log_{10} \left( \frac{T}{300} \right) - 2.163 \left[ \log_{10} \frac{T}{300} \right]^2$$

Let B denote a scale factor and let  $y_i$ ,  $i=1,7$  denote the normalized values of concentration. Define the quantities:

$$\begin{aligned}
X_1 &= By_1 = [RI] \\
X_2 &= By_2 = [R] \\
X_3 &= By_3 = [R_2] \\
X_4 &= By_4 = [I_2] \\
X_5 &= By_5 = [I^*] \\
X_6 &= By_6 = [I] \\
X_7 &= By_7 = \rho + (Z) \\
X_8 &= \rho - (Z) = K_0/X_7 \\
\rho &= \rho(Z) = X_7 + X_8
\end{aligned}$$

where  $[ ]$  denotes concentration of substance, R is the iodide perfluoride radical  $n\text{-C}_3\text{F}_7$ , I is iodine and  $I^*$  denotes the excited state of iodine. For  $w$  the flow rate of  $n\text{-C}_3\text{F}_7\text{I}$  in the Z direction (cm/sec) and  $\rho$  the total photon density, the differential equations defining the chemical kinetics of the amplifier are given by:



$$\omega \frac{dy_1}{dz} = K_1 By_2 y_5 + K_2 By_2 y_6 - \xi_1 y_1 - K_4 By_1 y_2 + K_5 By_2 y_4 - K_7 By_5 y_1 - K_6 By_2 y_1 - K_8 By_1 y_6 - y_1 \frac{d\omega}{dz}$$

$$\omega \frac{dy_2}{dz} = \xi_1 y_1 - K_1 By_2 y_5 - K_2 By_2 y_6 - 2K_3 By_2^2 - K_4 By_1 y_2 - K_6 By_1 y_2 - K_5 By_2 y_4$$

$$+ K_7 By_1 y_5 + K_8 By_1 y_6 - y_2 \frac{d\omega}{dz} - y_2 / r_2$$

$$\omega \frac{dy_3}{dz} = K_3 By_2^2 + K_6 By_1 y_2 + K_4 By_1 y_2 - y_3 \frac{d\omega}{dz} - y_3 / r_3$$

$$\omega \frac{dy_4}{dz} = C_1 B^2 y_1 y_5 y_6 + C_2 B^2 y_1 y_6^2 + C_3 B^2 y_4 y_5 y_6 + C_4 B^2 y_4 y_6^2 - \xi_2 y_4 + K_7 By_1 y_5$$

$$- K_5 By_2 y_4 + C_5 B^2 y_6^2 y_3 + K_8 By_6 y_1 + C_6 B^2 y_6 y_5 y_3 - y_4 \frac{d\omega}{dz} - y_4 / r_4$$

$$\omega \frac{dy_5}{dz} = \xi_1 y_1 + 0.51 \xi_2 y_4 - K_1 By_2 y_5 - C_1 B^2 y_1 y_5 y_6 - C_3 B^2 y_4 y_5 y_6 - Q_1 By_1 y_5 - Q_2 By_4 y_5$$

$$- C\sigma \cdot \rho \cdot (y_5 - \frac{1}{2} y_6) + K_6 By_2 y_1 - Q_3 By_5 y_2 - Q_4 By_5 y_3 - Q_5 By_5 y_6$$

$$- K_7 By_5 y_1 - C_6 B^2 y_6 y_5 y_3 - y_5 \frac{d\omega}{dz} - y_5 / r_5$$

$$\omega \frac{dy_6}{dz} = 1.49 \xi_2 y_4 + Q_1 y_1 y_5 + Q_2 By_4 y_5 - 2C_5 B^2 y_6^2 y_3 - K_8 By_6 y_1 + C\sigma \rho (y_5 - \frac{1}{2} y_6)$$

$$- C_1 B^2 y_1 y_5 y_6 - 2C_2 B^2 y_1 y_6^2 - C_3 B^2 y_4 y_5 y_6 - 2C_4 B^2 y_4 y_6^2 - K_2 By_2 y_6 + K_4 By_1 y_2$$

$$+ Q_3 By_5 y_2 + Q_4 By_5 y_3 + Q_5 By_5 y_6 + K_5 By_2 y_4 - C_6 B^2 y_6 y_5 y_3 - y_6 \frac{d\omega}{dz} - y_6 / r_6$$

$$\frac{dy_7}{dz} = L_c y_7 (y_5 - \frac{1}{2} y_6) B\sigma$$

Normalizing the length of the amplifier by using the substitution  $Z = SL$ ,  $0 < S < 1$  the differential equations are solved numerically using a Runge-Kutta integration scheme. Appendix A contains the computer code for the simulation of a two pass continuous wave amplifier. Appendix B contains a representation of the output from the code. This Appendix contains figures illustrating how concentrations change with distance. Current research is directed toward the refining of this program and performing a systems study with the parameters involved in the code construction.

**APPENDIX A**

**COMPUTER PROGRAM FOR SIMULATION OF TWO PASS CONTINUOUS WAVE AMPLIFIER**

PROGRAM TFAMP2(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE8)

MAIN PROGRAM

TWO PASS CONTINUOUS WAVE AMPLIFIER

AMPFAR IS THE DATA FILE WITH NAMELIST VARIABLES DEFINED

COMPRESSIBLE FLOW LASER MODEL WHICH INCLUDES

EQUATION OF STATE

CONTINUITY EQUATION

MOMENTUM EQUATION

ENERGY EQUATION

TAPE8 IS FOR OUTPUT DATA---RENAME AND SAVE TAPE8 IF YOU WANT  
TO SAVE THE OUTPUT DATA

PROBLEM IS SCALED IN THE AXIAL DIRECTION---LENGTH IS LC  
SCALED LENGTH IS ZERO TO ONE

SPECIFIC HEAT AT CONSTANT VOLUME IS FUNCTION OF TEMPERATURE  
OBTAINED FROM LEAST SQUARES FIT OF EMPIRICAL DATA  
FOR N-C3F7I IODINE LASER

USED IN PREDICTION MODE---GIVEN CONDITIONS AT Z=0.

THIS VERSION CONTAINS AN AUTOMATICALLY CHOSEN VARIABLE STEP  
SIZE. IT ALSO CONTAINS WALL EFFECT REACTIONS. (NOT USED THOUGH)

EFFECTS OF TEMPERATURE, FLOWRATE, DENSITY AND PRESSURE VARIATIONS  
ARE CONSIDERED IN SUBROUTINES ARREN, PFLOW AND FLOW

COMMON/BLK2/K1,K2,K3,K4,K5,K6,K7,K8,C1,C2,C3,C4,C5

COMMON/BLK27/Q1,Q2,Q3,Q4,Q5

COMMON/BLK3/B,B2,B3,C,A00,B00,EPSNU,OMEGA,C6

COMMON/BLK4/CHSI10,CHSI20,ABARO,Z1BAR,LC,XKO

COMMON/BLK7/ABC,C00,C0,OMEG1,P,R1,R2,TM,XNRHO

COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A,PIN,W

COMMON/BLK10/CF1,CF2,CF4,QFO,RSTAR,ZL,L,SF1,SF2,AR,AA0,BBO

COMMON/BLK22/AD,V1,V2,GG

COMMON/BLK23/W0,ETA0,PT0,FRAC

COMMON/BLK28/TAU2,TAU4,TAU5,TAU6,TAU3,SIG

COMMON/BLK299/TTT2,TTT3,TTT4,TTT5,TTT6

REAL K1,K2,K3,K4,K5,K6,K7,K8

REAL LC,L

WRITE(6,123)

123 FORMAT(1X,20H START OF PROGRAM )



```

ICOUNT=ICOUNT+1
READ(5,PARAM)
IF(EOF(5))600,601
600 WRITE(6,603)
603 FORMAT(1X,28HEND OF FILE ENCOUNTERED-STOP)
CALL PSEUDO
DO 10 JJJ=1,9
CALL GRAPHS(JJJ)
10 CONTINUE
STOP 1313

C
C W=TRANSMISSION COEFFICIENT
C PIN=INPUT POWER DENSITY (WATTS/CM**2)
C
C P=PRESSURE, TORR
C AP=LASER BEAM DIAMETER CM
C A=RADIUS OF TUBE (CM)
C RAD=RADIUS OF TUBE WHERE CALCULATIONS ARE DONE.
C T=TEMPERATURE DEG K
C TO=TEMPERATURE LEFT END DEG K
C PTO= PRESSURE TORR LEFT END
C WO=FLOW RATE LEFT END M/SEC
C ETAO=DENSITY OF GAS KG/M**3
C OMEG1=FLOW RATE, CM/SEC , MAXIMUM FLOW RATE AT RAD=0
C TAU2,TAU4,TAU5,TAU6 ARE LIFETIMES FOR RADIAL DIFFUSION OF
C TTT2,TTT3,TTT4,TTT5,TTT6 ARE LIFETIME VALUES FOR TAU
C THE QUANTITIES [R],[I2],[I*] AND [I].
C TAU3 IS DIFFUSION COEFFICIENT FOR [R2]
C CON=PEAK CONCENTRATION , SOLAR CONSTANTS
C COO=INITIAL GUESS AT RHO-PLUS AT ZERO
C WHICH IS SQUARE OF (COO*R1)
C R1= REFLECTIVITY AT LEFT END
C R2= REFLECTIVITY AT RIGHT END
C ZE=DISTANCE FOR LIGHT INTENSITY TO DIMINISH BY FACTOR 1/E
C TM= TRANSMISSION COEFFICIENT (OUTPUT MIRROR)
C ZOL=POINT ALONG AXIS WHERE MAXIMUM ILLUMINATION OCCURS
C IN THE CASE ILLUMINATION IS A BELL SHAPED CURVE
C IN THE CASE OF A SQUARE WAVE, 2*ZOL IS CUT OFF POINT
C THE POINT 2*ZOL IS WHERE ILLUMINATION BEGINS TO DIMINISH
C LC=LENGTH OF LASER CAVITY IN CM
C S= SCALED LENGTH WHICH GOES FROM ZERO TO ONE
C LENGTH IS SCALED FROM ZERO TO ONE
C ZL=2*ZOL LENGTH WHICH IS ILLUMINATED
C FRAC=FRACTION OF PEAK CONCENTRATION WHICH GOES
C INTO HEAT
C DEFAULT VALUE IS FRAC=0.024 I.E. 2.40 PERCENT
C H IS STEP SIZE FOR NUMERICAL INTEGRATION OVER SCALED LENGTH
C
601 CONTINUE
F=PTO
T=TO
ETAO=P*(1.01325E5)*296./(8314.3*760.*T)
C PTO IS PRESSURE IN TORR
C ETAO IS DENSITY IN KG/M**3
C ETAO IN KG/M**3

```

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```

C      F IN TORR
C      T IN DEG K
      CMIN=1.0E4
      CMAX=1.0E20
      ZL=2*ZOL
      L=LC
      CO=CON
      C11=CON
      CALL COEFFS
C      XO IN M/SEC
      XO=OMEGA/100.
C      OMEG1 AND OMEGA ARE IN CM/SEC
      WRITE(6,198)
198     FORMAT(///)
      WRITE(6,199) ZE,ZOL,CON,OMEGA,FRAC,COO,R1,R2,F,T
199     FORMAT(1X, T5,5HZE = ,F10.3,T30,6HZOL = ,E15.7,T55,6HCOO = ,
1 E15.7,T80,9HOMEGA = ,E15.7,T104,7HFRAC = ,F9.4,/,
2 1X,T5,6HCOO = ,E15.7, T30,6H R1 = ,F10.7, T55,6H R2 = ,F10.7,
3 T81,4H P = ,E15.7 ,T105,7HTEMP = ,F10.3)
C      SET UP COEFFICIENTS IN DIFFERENTIAL EQUATIONS
C      SET PRINTER OFF
C      IPRINT=0      PRINTER OFF
C      IPRINT=1      PRINTER ON
C      IPRINT=0
C      SET STEP SIZE H=.025 UNITS
      H=.025
C      INTEGRATE DIFFERENTIAL EQUATIONS FROM S=0 TO S=1.0
      X1=COO
      CALL INTEG(IPRINT,H)
C
C      INTERVAL HALVING SCHEME
C
      Y1=ABC
      IF(Y1.LT.0) PER=5.0
CC      IF(Y1.LT.0) PER=1.1
      IF(Y1.GT.0) PER=.1
CC      IF(Y1.GT.0) PER=.9
702     CONTINUE
C      IN THIS VERSION COO IS ASSUMED VALUE FOR RHO-(0)
      COO=(PER)*COO
      IF(COO .LT. CMIN) STOP 5432
      IF(COO .GT. CMAX) STOP 2345
      X2=COO
      CALL INTEG(IPRINT,H)
      Y2=ABC
C      ABC IS XKO INITIAL MINUS XKO CALCULATED (PERCENT ERROR)
      IF((Y1*Y2).LT. 0)GO TO 701
      X1=COO
      Y1=Y2
      GO TO 702
701     CONTINUE
      W1=.6
      W2=.4
      COO=W2*X1+W1*X2
708     CONTINUE
      CALL INTEG(IPRINT,H)

```

```

      X3=C00
      Y3=ABC
      IF (ABS(Y3).LT.0.05) GO TO 555
704  CONTINUE
      IF ((Y1*Y3).LT. 0) GO TO 705
C    Y1 & Y3 ARE OF THE SAME SIGN
      X1=X3
      Y1=Y3
      C00=.5*(X1+X2)
      GO TO 708
705  CONTINUE
C    Y1 & Y3 ARE OF OPPOSITE SIGN
      X2=X3
      Y2=Y3
      C00=.5*(X1+X2)
      GO TO 708
555  IPRINT=1
      --=0.025
      CALL INTEG(IPRINT,H)
      GO TO 55
END

```

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SUBROUTINE GRAPHS(JJJ)

AS THE NAME SUGGESTS THIS SUBROUTINE PLOTS GRAPHS OF THE  
NUMERICAL OUTPUT  
MULTIPLE PLOTS ON EACH GRAPH ---UP TO MAXIMUM OF EIGHT

```

COMMON/BLK4/CHSI10,CHSI20,ABARO,Z1BAR,LC,XK0
COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A,PIN,W
COMMON/BLK30/DATA(50,50),NDMAX,FLRATE(8),FDPTDAT(50,40)
DIMENSION X(50),Y(50),YY(50,8)
REAL LC

```

```

JJJ=1,9
JJJ=1 PLOT R VS Z
JJJ=2 PLOT I2 VS Z
JJJ=3 PLOT I* VS Z
JJJ=4 PLOT I VS Z
JJJ=5 PLOT INV VS Z
JJJ=6 PLOT FLOWRATE VS Z
JJJ=7 PLOT DENSITY VS Z
JJJ=8 PLOT PRESSURE VS Z
JJJ=9 PLOT TEMPERATURE VS Z

```

DATA ARRAY IS BY COLUMNS  
Z,R,I2,I\*,I,INV,Z,R,I2,I\*,I,INV,...  
ND=NUMBER OF DATA POINTS,=NUMBER OF ROWS IN DATA ARRAY  
NG=NUMBER OF CURVES PER GRAPH



```

C      IC IS CODE TO DETERMINE NUMBER OF GRAPHS TO PLOT
C      IC=0 FOR MORE THAN ONE GRAPH
C      IC=1 FOR LAST GRAPH (USED FOR ONLY ONE GRAPH)
C
C      IC=0
C      NLAST=NG-1
C      SXC=5.0
C      SYC=5.0
C      SYCI=7.0
C      SXC=LENGTH OF XSCALE
C      SYC=LENGTH OF YSCALE
C      SYCI=LENGTH OF YSCALE FOR INVERSION
C      IF(NLAST .EQ. 0) IC=1
C      PLOT JJJ VS Z
C      IF(JJJ .GE. 6) GO TO 700
C      DO 10 I=1,NDMAX
C      X(I)=DATA(I,1)
C      DO 20 J=1,NG
C      NN=(J-1)*6
C      NCOL=NN+1+JJJ
C      YY(I,J)=DATA(I,NCOL)
20    CONTINUE
60    CONTINUE
C
C      FIND YMAX,YMIN
C
C
C      DMAX=0.0
C      YMAX=0.0
C      YMIN=0.0
C      ZMIN=0.0
C
C      FIND YMAX AND YMIN
C
C      DO 70 I=1,NDMAX
C      DO 71 J=1,NG
C      IF( YY(I,J) .GT. YMAX) YMAX=YY(I,J)
C      IF( YY(I,J) .LT. YMIN) YMIN=YY(I,J)
71    CONTINUE
70    CONTINUE
C
C      PLOT FIRST DATA CURVE
C
C      JJJ=1
C      ZMAX=1.00
C      DO 40 I=1,NDMAX
C      Y(I)=YY(I,1)
40    CONTINUE
C      LOGMAX=1+ALOG10(ABS(YMAX))
C      POWER1=10.**LOGMAX
C      TEST=YMAX/POWER1
C      YMAXX=0.025
C      IF(TEST .GT. 0.025) YMAXX=.05
C      IF(TEST .GT. 0.05) YMAXX=0.10
C      IF(TEST .GT. 0.10) YMAXX=0.25

```

```

IF (TEST .GT. 0.25) YMAXX=0.50
IF (TEST .GT. 0.5) YMAXX=1.00
YMAX=YMAXX*POWER1
IF (JJJ.NE. 5) GO TO 507
506 CONTINUE
IF (YMIN .GE. 0) GO TO 507
IF (YMIN .LT. 0.0) LOGMAX2=1+ALOG10 (ABS (YMIN))
POWER=10.**LOGMAX2
TEST=ABS (YMIN)/POWER
YMINN=0.001
IF (TEST .GT. 0.001) YMINN=0.005
IF (TEST .GT. 0.005) YMINN=0.01
IF (TEST .GT. 0.01) YMINN=0.05
IF (TEST .GT. 0.05) YMINN=0.1
IF (TEST .GT. 0.10) YMINN=0.5
IF (TEST .GT. 0.5) YMINN=1.0
YMIN=-YMINN*POWER
SYC=SYCI
507 CONTINUE
ZMIN=0.0
IF (JJJ.GT.1) GO TO 50
C
C JJJ=1 PLOT R VS Z
CALL INFOPLT (IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1 22,22HZ, SCALE DISTANCE,
2 11,11H [C3F7] ,0,
3 SXC,SYC,0.75,0.75)
GO TO 600
50 CONTINUE
IF (JJJ.GT.2) GO TO 100
C
C JJJ=2 PLOT I2 VS Z
CALL INFOPLT (IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1 23,23HZ, SCALE DISTANCE,
2 9,9H [I2] ,0,
3 SXC,SYC,0.75,0.75)
GO TO 600
100 CONTINUE
IF (JJJ.GT.3) GO TO 200
C
C JJJ=3 PLOT I* VS Z
CALL INFOPLT (IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1 23,23HZ, SCALE DISTANCE,
2 9,9H [I*] ,0,
3 SXC,SYC,0.75,0.75)
GO TO 600
200 CONTINUE
IF (JJJ.GT.4) GO TO 300
C
C JJJ=4 PLOT I VS Z
CALL INFOPLT (IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1 23,23HZ, SCALE DISTANCE,
2 8,8H [I] ,0,

```

```

3   SXC,SYC,0.75,0.75)
    GO TO 600
300  CONTINUE
C
C   JJJ=5   PLOT INV VS Z
C
    CALL INFOFLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1   23,23HZ, SCALE DISTANCE,
2   24,24H      [I*]-.5*[II] ,0,
3   SXC,SYC,0.75,0.75)
600  CONTINUE
C   PLOT REST OF CURVES OR EXIT IF ONLY ONE CURVE
C
    NLAST=NG-1
    IF(NG .EQ. 2) GO TO 5001
    IF(NLAST .EQ. 0) GO TO 601
    DO 500 J=2,NLAST
    DO 501 I=1,NDMAX
    Y(I)=YY(I,J)
501  CONTINUE
    CALL INFOFLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1   1,1H ,1,1H ,0,SXC,SYC,0.75,0.75)
500  CONTINUE
5001  CONTINUE
C
C   PLOT LAST CURVE
C
    DO 60 I=1,NDMAX
    Y(I)=YY(I,NG)
60  CONTINUE
    CALL INFOFLT(1,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1   1,1H ,1,1H ,0,SXC,SYC,0.75,0.75)
601  CONTINUE
    CALL NFRAME
    RETURN
700  CONTINUE
C   GET DATA TO PLOT
    DO 701 I=1,NDMAX
    X(I)=FDPTDAT(I,1)
    DO 702 J=1,NG
    NN=JJJ-4+(J-1)*5
    YY(I,J)=FDPTDAT(I,NN)
702  CONTINUE
C   FDPTDAT IS STORED IN THE FORM:
C   Z, FLOWRATE, DENSITY, PRESSURE, TEMPERATURE, Z, FLOWRATE, ...
701  CONTINUE
C   FIND MAX AND MIN FOR Y VALUES
    YMIN=100.
    YMAX=0.0
    DO 703 I=1,NDMAX
    DO 704 J=1,NG
    IF(YY(I,J) .LT. YMIN) YMIN=YY(I,J)
    IF(YY(I,J) .GT. YMAX) YMAX=YY(I,J)
704  CONTINUE
703  CONTINUE
    MAX=10.*YMAX+1.0

```

```

      YMAX=FLOAT(MAX)/10.
      MIN=10.*YMIN-1.0
      YMIN=FLOAT(MIN)/10.
      ZMIN=0.0
      ZMAX=1.0
C      PLOT FIRST CURVEC
      DO 705 I=1,NDMAX
      NN=1
705   Y(I)=YY(I,NN)
C      PLOT JJJ VS Z
      IF(JJJ .GT. 6) GO TO 800
C      JJJ=6, PLOT FLOWRATE VS Z
      CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1 25,25HZ, AXIAL DISTANCE, SCALED ,
2 15,15FLOWRATE CM/SEC      , 0 ,
3 10.,5.,0.75,0.75)
      GO TO 820
800   CONTINUE
      IF(JJJ .GT. 7) GO TO 801
C      JJJ=7, PLOT DENSITY VS Z
      CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1 25,25HZ, AXIAL DISTANCE, SCALED ,
2 16,16HDENSITY, KG/M**3      , 0 ,
3 10.,5.,0.75,0.75)
      GO TO 820
801   CONTINUE
      IF(JJJ .GT. 8) GO TO 802
C      JJJ=8, PLOT PRESSURE VS Z
      CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1 25,25HZ, AXIAL DISTANCE, SCALED ,
2 14,14HPRESSURE, TORR      , 0 ,
3 10.,5.,0.75,0.75 )
      GO TO 820
802   CONTINUE
C      JJJ=9, PLOT TEMPERATURE VS Z
      CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1 25,25HZ, AXIAL DISTANCE, SCALED ,
2 18,18HTEMPERATURE, DEG C      , 0 ,
3 10.,5.,0.75,0.75 )
820   CONTINUE
      IF(NLAST .EQ. 0) GO TO 901
C      PLOT REST OF THE CURVES
      IF(NG .EQ. 2) GO TO 5031
      DO 503 J=2,NLAST
      DO 504 I=1,NDMAX
      NN=J
      Y(I)=YY(I,NN)
504   CONTINUE
      CALL INFOPLT(IC,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1 1,1H ,1,1H ,0,10.,5.,0.75,0.75 )
503   CONTINUE
5031  CONTINUE
C      PLOT LAST CURVE
      DO 505 I=1,NDMAX
      Y(I)=YY(I,NG)
505   CONTINUE

```

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OF POOR QUALITY

```

CALL INFOPLT(1,NDMAX,X,1,Y,1,ZMIN,ZMAX,YMIN,YMAX,1.0,
1 1,1H ,1,1H ,0,10.,5.,0.75,0.75 )
901 CONTINUE
CALL NFRAME
RETURN
END

SUBROUTINE PFLOW
C SUBROUTINE TO CALCULATE THE PARAMETERS FOR SUBROUTINE FLOW
C PARAMETERS STORE IN COMMON BLK10
COMMON/BLK7/ABC,C00,C0,OMEG1,P,R1,R2,TM,XNRHO
COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A,PIN,W
COMMON/BLK10/CF1,CF2,CF4,QFO,RSTAR,ZL,L,SF1,SF2,AR,AAO,BBO
COMMON/BLK23/WO,ETA0,PT0,FRAC
COMMON/BLK29/ ZZZ,TZZ,PZZ,ETAZZ,WZZ
REAL L

C
C AR IS BEAM DIAMETER RADIUS IN CM
SF1=1000./296.
C SF1 =1/(M*1.E-03), WHERE M IS THE MOLECULAR WEIGHT
C CVS (J/K KG) =SF1*CV (J/K MOL)
SF2=(1.01325E5)/760.
C SF2 EQUALS 133.3 PA/TORR
C SF1,SF2 ARE SCALE FACTORS FOR THE CORRECT UNITS OF
C P=PRESSURE (N/M**2) , SF1 (MOLE/KG)
C PT=PRESSURE (TORR), SF2 (N/M**2)/TORR
C TEST TO SEE IF WO (M/SEC) IS NEAR MAX VALUE OF 5.30*SQRT(TO)
TEST=5.3*SQRT(TO)
TEST1=ABS(100.*(WO-TEST)/TEST)
IF(TEST1 .LT. 10.0) WRITE(6,778)
778 FORMAT(1X,52HWARNING WO VALUE IS WITHIN 10 PERCENT OF ITS MAXIMUM
1 ,/,1X,35HALLOWABLE VALUE OF 5.3*SQRT(TO) )
C ZL=LIGHT SOURCE LENGTH IN CM
C ETA=DENSITY (KG/M**3)
C L=TUBE LENGTH IN CM
C RSTAR=GAS CONSTANT (JOULE/KG DEG K)
C T=TEMPERATURE (DEG K)
C CV=SPECIFIC HEAT AT CONSTANT VOLUME
C RSTAR (J/K KG) = SF1*R(J/K MOL)
C WO,WL=FLOW VELOCITY (M/SEC) (SUBSCRIPTS O,L FOR START,END)
PO=SF2*PT0
RSTAR=8314.3/296.0
CF1=ETA0*WO
CF2=CF1*WO+PO
QFO=FRAC*(1.40E3)*C0 *2./(A*1.E-2)
C QFO IN W/M**3
C INPUT (W/M**2) DISTRIBUTED OVER VOLUME (2*(PI)*A)/PI(A**2) IN M2/M3
WZZ=WO
RETURN
END

SUBROUTINE FLOW(Z,T,PTORR,WSS,ETA,DWDZ)

```

```

COMMON/BLK8/ZOL, ZE, NG, TO, RAD, A, PIN, W
C SUBROUTINE TO CALCULATE T, P, WSS, ETA AS FUNCTION OF Z
COMMON/BLK10/CF1, CF2, CF4, QFO, RSTAR, ZL, L, SF1, SF2, AR, AAO, BBO
COMMON/BLK23/WO, ETAO, PTO, FRAC
C
COMMON/BLK29/ ZZZ, TZZ, PZZ, ETAZZ, WZZ
REAL L
ICOUNT=0
Q=QFO*Z/100.
C ENERGY INPUT TERM DETERMINED BY QFO
C Z IS IN CM AND QFO IS IN W/M**3
IF (Z.GT.ZL) Q=QFO*ZL/100.
XXX=BBO*(TO-300.)
CALL ETO (XXX, EEO)
WSS=WZZ
50 CONTINUE
T=((CF2/CF1)*WSS-WSS*WSS)/RSTAR
DTDW=((CF2/CF1)-2.*WSS)/RSTAR
XXX=BBO*(T-300.)
CALL ETO (XXX, EE1)
F=RSTAR*(T-TO)+(AAO/BBO)*SF1*(EE1-EEO)+
1 .5*(WSS*WSS-WO*WO)-Q/CF1
FP=(RSTAR+SF1*AAO*EE1)*DTDW+WSS
W1=WSS-F/FP
ERR=ABS(100.*(W1-WSS)/WSS)
IF (ERR .LT. .25) GO TO 100
IF (ICOUNT .GT. 95) WRITE (6, 357) ICOUNT, Z, WZZ, WSS, CF1, CF2, TO, Q, FM
357 FORMAT (1X, I5, 1X, (3E16.7, /))
WSS=W1
ICOUNT=ICOUNT+1
IF (ICOUNT .GT. 100) STOP 4444
GO TO 50
100 CONTINUE
WSS=W1
T=((CF2/CF1)*WSS-WSS*WSS)/RSTAR
TC=T-273
ETA=CF1/WSS
PNM2=ETA*RSTAR*T
PTORR=PNM2/SF2
ZZZ=Z
TZZ=TC
PZZ=PTORR
ETAZZ=ETA
WZZ=WSS
XXX=BBO*(T-300.)
CALL ETO (XXX, CVO)
CV=CVO*AAO
CVS=SF1*CV
XNUM=RSTAR*QFO
XDEN=(CF2-2.*CF1*WSS)*(CVS+RSTAR)+RSTAR*CF1*WSS
DWDZ=XNUM/XDEN
RETURN
END

```

SUBROUTINE ARREN(TEMP)

SUBROUTINE FOR ARRENIUS EXPRESSION OF RATE COEFFICIENTS

BASIC ASSUMPTIONS

FOR QI TERMS  $QI=QIO*EXP(-BETA*(TEMP-TO))$

TREAT KI TERMS LIKE CI TERMS

COMMON/BLK2/K1,K2,K3,K4,K5,K6,K7,K8,C1,C2,C3,C4,C5

COMMON/BLK27/Q1,Q2,Q3,Q4,Q5

COMMON/BLK3/B,B2,B3,C,A00,B00,EPSNU,OMEGA,C6

COMMON/BLK11/KK1, KK2, KK3, KK4, KK5, KK6, KK7, KK8

COMMON/BLK12/QQ1, QQ2, QQ3, QQ4, QQ5

COMMON/BLK13/CC1, CC2, CC3, CC4, CC5, CC6

REAL K1,K2,K3,K4,K5,K6,K7,K8, KK1, KK2, KK3, KK4, KK5, KK6, KK7, KK8

REFERENCE J.S. COHEN AND O.P. JUDD

J.APPL. PHYS., VOL 55, NO. 7, APRIL 1984

COEFFICIENTS MODIFIED TO ACHIEVE SPECIFIC VALUES AT TEMPERATURE  
OF 276 DEGREES K.

BETA=4.4E-3

SF1=1.0

XXX=-BETA\*(TEMP-300)

CALL ETO(XXX,YYY)

SF2=YYY

K1=KK1\*SF1

K2=KK2\*SF1

K3=KK3\*SF1

K4=KK4\*SF1

K5=KK5\*SF1

K6=KK6\*SF1

K7=KK7\*SF1

K8=KK8\*SF1

C1=CC1\*SF1

C2=CC2\*EXP(1360.00/TEMP)

C3=CC3\*SF1

XYZ=-29.437-5.844\*ALOG10(TEMP/300.)+2.163\*(ALOG10(TEMP/300.))\*\*2

C4=CC4\*\*XYZ

C5=CC5\*EXP(1310.000/TEMP)

C6=CC6\*SF1

Q1=QQ1\*SF1

Q2=QQ2\*EXP((-4.4E-3)\*(TEMP-300.))

Q3=QQ3\*SF1

Q4=QQ4\*SF1

Q5=QQ5\*SF1

RETURN

END

SUBROUTINE ETO(X,Y)

NEGATIVE EXPONENTIAL FUNCTION

IF(X.LT. -670.) GO TO 100

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```

      Y=EXP(X)
      RETURN
100   Y=0.
      RETURN
      END

```

```

      FUNCTION CHSI1(Z)
      C      Z1BAR IS CUTOFF POINT OF ILLUMINATION
      C      ABARO IS FRONT CUTOFF POINT OF ILLUMINATION
      C      CHSI1 IS A CONSTANT
      C      IMPLICIT REAL*8(A-H,K,L,O-Z)
      COMMON/BLK4/CHSI10,CHSI20,ABARO,Z1BAR,LC,XKO
      COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A,PIN,W
      REAL LC
      IF(Z.LT.ABARO) GO TO 100
      IF(Z.LT.Z1BAR) GO TO 200
      C      Z GREATER THAN Z1BAR
100   CHSI1=0.0
      C      CHSI1 HAS UNITS OF SEC^-1
      RETURN
200   CONTINUE
      CHSI1=CHSI10
      RETURN
      END

```

```

      FUNCTION CHSI2(Z)
      C      ABARO IS FRONT CUTOFF POINT FOR ILLUMINATION
      C      Z1BAR IS CUTOFF POINT FOR ILLUMINATION
      C      CHSI2 IS A CONSTANT
      C      IMPLICIT REAL*8(A-H,K,L,O-Z)
      COMMON/BLK4/CHSI10,CHSI20,ABARO,Z1BAR,LC,XKO
      COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A,PIN,W
      REAL LC
      IF(Z.LT.ABARO) GO TO 100
      IF(Z.LT.Z1BAR) GO TO 200
      C      Z GREATER THAN Z1BAR
      CC      XXX=-(Z-Z1BAR)/ZE
      CC      CALL ETO(XXX,YYY)
      CC      CHSI2=CHSI20*YYY
      C      CHSI2 HAS UNITS OF SEC^-1
      RETURN
100   CHSI2=0.0
      RETURN
200   CONTINUE
      CHSI2=CHSI20
      RETURN
      END

```



SUBROUTINE COEFFS

# COEFFICIENTS IN THE DIFFERENTIAL EQUATIONS

$$AEAR_0 = 0,0$$
[illegible]

```

C      (Q01)      I* + RI --> I + RI
C      (Q02)      I* + I2 --> I + I2
C      (Q03)      I* + R  --> I + R
C      (Q04)      I* + R2 --> I + R2
C      (Q05)      I* + I  --> I + I
C
CC      (CC1)      I* + I + RI --> I2 + R1
CC      (CC2)      I + I + RI --> I2 + RI
CC      (CC3)      I* + I + I2 --> I2 + I2
CC      (CC4)      I + I + I2 --> I2 + I2
CC      (CC5)      I + I + R2 --> I2 + R2
CC      (CC6)      I + I* + R2 --> I2 + R2

```

# WALL REACTIONS

```

C      (V1)      I + I + WALL --> I2 + WALL
C      (V2)      R2 + I + WALL --> R + RI + WALL

```

```

C      CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC

```

```

C      WILSON ET AL. (1984) AND STOCK ET AL. (1986)
C      KK1 = 5.6E-13
C      COHEN AND JUDD (1984)
C      KK1 = .9E-13
C      VINOKKUROV AND ZALESSKKII (1979)
C      KK1 = 1.E-14

```

```

C      WILSON ET AL. (1984) AND STOCK ET AL. (1986)
C      KK2 = 2.3E-11
C      BREDERLOW ET AL. (1983)
C      KK2 = .8E-11
C      COHEN AND JUDD (1984)
C      KK2 = .7E-11

```

```

C      WILSON ET AL. (1984) AND STOCK ET AL. (1986)
C      KK3 = 2.6E-12
C      BREDERLOW ET AL. (1983) AND COHEN AND JUDD (1984)
C      KK3 = 2.0E-12

```

```

C      WILSON ET AL. (1984), STOCK ET AL. (1986), AND COHEN AND JUDD (1984)
C      KK4 = 3.E-16

```

```

C      COHEN AND JUDD (1984)
C      KK5 = 1.0E-11

```

```

C      WILSON ET AL. (1984) AND STOCK ET AL. (1986)
C      KK6 = 3.2E-17

```

```

C BREDERLOW ET AL. (1983) AND COHEN AND JUDD (1984)
  KK6 = 0.
C
C
C COHEN AND JUDD (1984)
  KK7 = 3.0E-19
C
C
C
C COHEN AND JUDD (1984)
  KK8 = 1.6E-23
C
C
C WILSON ET AL. (1984) AND STOCK ET AL. (1986)
  QQ1 = 2.0E-16
C COHEN AND JUDD (1984)
  QQ1 = 1.7E-16
C BREDERLOW ET AL. (1983)
  QQ1 = 1.7E-17
C
C
C
C COHEN AND JUDD (1984)
  QQ2 = 3.80E-11*EXP(-4.4E-3*(T-300.))
  QQ2=3.8E-11
C SUBROUTINE ARREN ADDS TEMPERATURE EFFECT
C BREDERLOW ET AL. (1983)
  QQ2 = 3.0E-11
C WILSON ET AL. (1984) AND STOCK ET AL. (1986)
  QQ2 = 1.9E-11
C
C
C
C COHEN AND JUDD (1984)
  QQ3 = 3.7E-18
C
C
C COHEN AND JUDD (1984)
  QQ4 = 4.7E-16
C
C
C COHEN AND JUDD (1984)
  QQ5 = 1.6E-14
C
C
C
C COHEN AND JUDD (1984) (A DIFFERENT REACTION, PERHAPS)
CC CC1 = 1.E-32
CC WILSON ET AL. (1984) AND STOCK ET AL. (1986)
CC CC1 = 3.2E-33
CC HOHLA AND KOMPA (1976)
CC CC1 = 1.6E-33
CC
CC
C COHEN AND JUDD (1984)
C CC2 = 5.7E-33*EXP(1360./T)

```

```

      CC2 = 5.7E-33
C      SUBROUTINE ARREN ADDS TEMPERATURE EFFECT
CC      HOHLA AND KOMPA (1976)
CC      CC2 = 2.1E-33*EXP(1600./T)
C      BREDERLOW ET AL. (1983)
CC      CC2 = 3.8E-31
C      WILSON ET AL. (1984) AND STOCK ET AL. (1986)
CC      CC2 = 8.5E-32
C
C
C      WILSON ET AL. (1984) AND STOCK ET AL. (1986)
CC      CC3 = 8.E-32
C      BREDERLOW ET AL. (1983) AND COHEN AND JUDD (1984)
      CC3 = 0.
C
C
C      WILSON ET AL. (1984) AND STOCK ET AL. (1986)
CC      CC4 = 3.8E-30
C      COHEN AND JUDD (1984)
C      CC4 = 10.0**(-29.437-5.844*ALOG10(T/300.))
      CC4 = 10.0
C      SUBROUTINE ARREN ADDS TEMPERATURE EFFECT
C      BREDERLOW ET AL. (1983)
CC      CC4 = 2.9E-30
C
C
C      COHEN AND JUDD (1984)
C      CC5 = 8.E-33*EXP(1310./T)
      CC5 = 8.0E-33
C      SUBROUTINE ARREN ADDS TEMPERATURE EFFECT
C
C
C      BREDERLOW ET AL. (1983) AND COHEN AND JUDD (1984)
      CC6 = 0.0
C
C
C      V1 = 0.0
C
C
C      V2 = 0.0
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C
C      KK1=.903E-13
C      KK2=80.E-12
C      KK3=.65E-12
C      KK4=1.000E-16
C      KK5=3.089E711
C      KK7=.1517E-18
C      KK8=1.6E-23
C
C      QQ1=.476E-16
C      QQ2=1.9E-11
C      QQ3=.1235E-17
C      QQ4=1.57E-16

```

```

C      Q05=.53E-14
C
CC      CC1=1.053E-33
CC      CC2=45.0E-32
CC      CC3=.4447E-31
CC      CC4=4.94E-30
CC      CC5=3.6E-31
CC      CC6=      1.8E-32
C
C      V1=      1.0E-12
C      V2=      1.0E-11
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C

```

```

      GG=2*(.18/LC)**2
      C=3.0E10
CC      B=P*(3.5E16)
      B=(9.66E18)*P/TO
      B2=B*B
      B3=B2*B
      RETURN
      END

```

```

C      SUBROUTINE VELOC(OMEG1,RAD,OMEGA,A)
C      VELOCITY PROFILE IS ASSUMED TO BE PARABOLIC
C      MAX VELOCITY AT RAD=0.0
C      ZERO VELOCITY AT RAD=A
C      A IS RADIUS OF TUBE
C      OMEG1 IS MAXIMUM VELOCITY ALONG CENTERLINE
C
C      CALCULATE VELOCITY OMEGA AT R=RAD
C      0 .LE. RAD .LE. A
C
C      TYPE OF FLOW
C      OMEGA=(OMEG1/(A*A))*(RAD-A)**2
C      RETURN
C      END

```

```

      SUBROUTINE PRINT(Z,TEMP)
COMMON/BLK2/K1,K2,K3,K4,K5,K6,K7,K8,C1,C2,C3,C4,C5
COMMON/BLK27/Q1,Q2,Q3,Q4,Q5
COMMON/BLK3/B,B2,B3,C,A00,B00,EPSNU,OMEGA,C6
COMMON/BLK4/CHSI10,CHSI20,ABARO,Z1BAR,LC,XKO
COMMON/BLK7/ABC,C00,C0,OMEG1,P,R1,R2,TM,XNRHO
COMMON/BLK22/AD,V1,V2,GG

```

```

COMMON/BLK28/TAU2,TAU4,TAU5,TAU6,TAU3,SIG
COMMON/BLK299/TTT2,TTT3,TTT4,TTT5,TTT6
REAL K1,K2,K3,K4,K5,K6,K7,K8,LC

```

```

C
  IF(Z .EQ. 0.0) WRITE(6,10)
10  FORMAT(1X,20HCOEFFICIENTS AT Z=0      )
  IF(Z .GE. 1.0) WRITE(6,11)
11  FORMAT(1X,20HCOEFFICIENTS AT Z=L      )
C    WRITE OUT COEFFICIENTS
      WRITE(6,100) K1,K7,Q1,C5,TTT2
      WRITE(6,101) K2,K8,Q2,V1,TTT3
      WRITE(6,102) K3,C1,Q3,V2,TTT4
      WRITE(6,103) K4,C2,Q4,SIG,TTT5
      WRITE(6,104) K5,C3,Q5,TEMP,TTT6
      WRITE(6,105) K6,C4,C6,LC
100  FORMAT(T5,5HKK1 = ,E15.7,T30,5HKK7 = ,E15.7,T60,5HQ01 = ,E15.7 ,
1    T85,5HCC5 = ,E15.7 , T103,7HTTT2 = ,E15.7 )
101  FORMAT(T5,5HKK2 = ,E15.7,T30,5HKK8 = ,E15.7,T60,5HQ02 = ,E15.7 ,
1    T85,5HV1 = ,E15.7 , T103,7HTTT3 = ,E15.7 )
102  FORMAT(T5,5HKK3 = ,E15.7,T30,5HCC1 = ,E15.7,T60,5HQ03 = ,E15.7 ,
1    T85, 5HV2 = ,E15.7 , T103,7HTTT4 = ,E15.7 )
103  FORMAT(T5,5HKK4 = ,E15.7,T30,5HCC2 = ,E15.7,T60,5HQ04 = ,E15.7 ,
1    T85, 8HSIGMA = ,E15.7 , T103,7HTTT5 = ,E15.7 )
104  FORMAT(T5,5HKK5 = ,E15.7,T30,5HCC3 = ,E15.7,T60,5HQ05 = ,E15.7 ,
1    T85,7HTEMP = ,F9.2 , T103,7HTTT6 = ,E15.7 )
105  FORMAT(T5,5HKK6 = ,E15.7,T30,5HCC4 = ,E15.7,T60,5HCC6 = ,E15.7 ,
1    T85, 4HL = ,F9.2 )
      RETURN
      END

```

```

SUBROUTINE FUN(N,S,Y,F)

```

```

C    THIS SUBROUTINE DEFINES THE RIGHT HAND SIDE
C    OF THE DIFFERENTIAL EQUATIONS FOR THE CHEMICAL KINETICS
C    IMPLICIT REAL*8(A-H,K,L,O-Z)
      DIMENSION Y(7),F(7)
      COMMON/BLK1/X7,POWER
      EXTERNAL CHSI1,CHSI2
      COMMON/BLK2/K1,K2,K3,K4,K5,K6,K7,K8,C1,C2,C3,C4,C5
      COMMON/BLK27/Q1,Q2,Q3,Q4,Q5
      COMMON/BLK3/B,B2,B3,C,A00,B00,EPSNU,OMEGA,C6
      COMMON/BLK4/CHSI10,CHSI20,ABAR0,Z1BAR,LC,XK0
      COMMON/BLK7/ABC,C00,C0,OMEG1,F,R1,R2,TM,XNRHO
      COMMON/BLK22/AD,V1,V2,G6
      COMMON/BLK28/TAU2,TAU4,TAU5,TAU6,TAU3,SIG
      COMMON/BLK299/TTT2,TTT3,TTT4,TTT5,TTT6
      REAL K1,K2,K3,K4,K5,K6,K7,K8,LC

```

```

C
C    QY=QUANTUM YIELD
C    QY=1.0
C
C    F(I),I=1,6 ARE RATES OF CHANGES FOR THE CONCENTRATIONS
C    F(1)=D[R1]/DZ      F(2)=D[R1]/DZ
C    F(3)=D[R2]/DZ      F(4)=D[I2]/DZ
C

```

```

C          F(5)=D[I*]/DZ          F(6)=D[I]/DZ
C
20  CONTINUE
    Z=LC*S
C    S IS SCALED LENGTH VARIABLE
C    O .LE. S .LE. 1
C    FLOW CALCULATES TEMPERATURE, PRESSURE, FLOWRATE
C    AND DENSITY RESPONSE AS FUNCTION OF Z
C
C    Z IS DISTANCE IN CM
C    CALCULATE GAS PARAMETERS AS FUNCTION OF Z
C    CALL FLOW(Z,TEMP,PRESS,FLOWR,DENSITY,DWDZ)
C    CALL FLOW(Z,TEMP,PRESS,FLOWR,DENSITY,DWDZ)
C    WRITE(6,357)Z,TEMP,PRESS,FLOWR,DENSITY,DWDZ
357  FORMAT(1X,3E16.7,/,3E16.7 )
C    TEMP IS TEMPERATURE DEG K
C    PRESS IS PRESSURE IN TORR
C    FLOWR IS FLOWRATE IN M/SEC
C    DENSITY IS GAS DENSITY IN KG/M**3
C    OMEGA=FLOWR*100.
C    OMEGA IS FLOW RATE IN CM/SEC
C    CALCULATE COEFFICIENTS AS FUNCTION OF TEMP AND Z
C    CALL ARREN(TEMP)
C    TAU5=(TTT5)*PRESS
C    TAU6=TAU5
C
C
C    CONSTANTS COME VIA COMMON BLKS 2 AND 3
C    K'S IN CM**3/SEC
C    C'S IN CM**6/SEC
C    Q'S IN CM**3/SEC
C    R0W0R0I5YI0W0CM**2
C    X7STAR=Y(7)*B+X8
C    DIF=Y(5)-.5*Y(6)
C    CALL SIGMA(SIG2)
C    SIG=SIG2
C    F(1)=K1*B*Y(2)*Y(5)+K2*B*Y(2)*Y(6)-CHSI1(Z)*Y(1)-K4*B*Y(1)*Y(2)
1    +K5*B*Y(2)*Y(4) -K7*B*Y(5)*Y(1)-K6*B*Y(2)*Y(1) +V2*B*Y(3)*Y(6)
2    -K8*B*Y(6)*Y(1) -Y(1)*DWDZ
C    F(2)=CHSI1(Z)*Y(1)-K1*B*Y(2)*Y(5)-K2*B*Y(2)*Y(6)-2*K3*B*Y(2)*Y(2)
1    -K4*B*Y(1)*Y(2)-K6*B*Y(1)*Y(2)-K5*B*Y(2)*Y(4)+V2*B*Y(3)*Y(6)
2    +K7*B*Y(5)*Y(1) +K8*B*Y(6)*Y(1) -Y(2)*DWDZ-Y(2)/TAU2
C    F(3)=K3*B*Y(2)*Y(2)+K6*B*Y(1)*Y(2)+K4*B*Y(1)*Y(2)-V2*B*Y(3)*Y(6)-
1    Y(3)*DWDZ -Y(3)/TAU3
C    A1=C1*B2*Y(1)*Y(5)*Y(6)+C2*B2*Y(1)*Y(6)*Y(6)+C3*B2*Y(4)*Y(5)*Y(6)
C    A2=C4*B2*Y(4)*Y(6)*Y(6)-CHSI2(Z)*Y(4)+K7*B*Y(5)*Y(1)
1    -K5*B*Y(2)*Y(4) +V1*B*Y(6)*Y(6) +C5*B2*Y(6)*Y(6)*Y(3)
C    F(4)=A1+A2+K8*B*Y(6)*Y(1)+C6*B2*Y(6)*Y(5)*Y(3)-Y(4)*DWDZ-Y(4)/TAU4
C    A3=QY*CHSI1(Z)*Y(1)+0.51*CHSI2(Z)*Y(4)-K1*B*Y(2)*Y(5)
C    A4=-C1*B2*Y(1)*Y(5)*Y(6)-C3*B2*Y(4)*Y(5)*Y(6)-Q1*B*Y(1)*Y(5)
C    A5=-Q2*B*Y(4)*Y(5)-C*SIG*X7STAR*DIF +K6*B*Y(2)*Y(1)
C    F(5)=A3+A4+A5-Q3*B*Y(5)*Y(2)-Q4*B*Y(5)*Y(3)-Q5*B*Y(5)*Y(6)
1    -K7*B*Y(5)*Y(1)-C6*B2*Y(6)*Y(5)*Y(3)-Y(5)*DWDZ-Y(5)/TAU5
C    A6=1.49*CHSI2(Z)*Y(4)+Q1*B*Y(1)*Y(5)+Q2*B*Y(4)*Y(5)
1    -2*C5*B2*Y(6)*Y(6)*Y(3) -K8*B*Y(6)*Y(1)
C    A7=C*SIG*X7STAR*DIF -C1*B2*Y(1)*Y(5)*Y(6)

```

```

A8=-2*C2*B2*Y(1)*Y(6)*Y(6)-C3*B2*Y(4)*Y(5)*Y(6)
A9=-2*C4*B2*Y(4)*Y(6)*Y(6)-K2*B*Y(2)*Y(6)+K4*B*Y(1)*Y(2)
A10=Q3*B*Y(5)*Y(2)+Q4*B*Y(5)*Y(3)+Q5*B*Y(5)*Y(6)
1 +K5*B*Y(2)*Y(4) -V2*B*Y(3)*Y(6) -2*V1*B*Y(6)*Y(6)
F(6)=A6+A7+A8+A9+A10-C6*B2*Y(6)*Y(5)*Y(3) -Y(6)*DWDZ-Y(6)/TAU6
C   SCALED EQUATIONS IN THE Z-DIRECTION
DO 10 I=1,6
10  F(I)=LC*F(I)/OMEGA
    F(7)=LC*Y(7)*DIF*B*SIG
    RETURN
END

```

```

C   SUBROUTINE SIGMA(SIG)
    THIS SUBROUTINE DEFINES THE CROSS SECTION SIGMA
COMMON/BLK3/B, B2, B3, C, A00, B00, EPSNU, OMEGA, C6
COMMON/BLK7/ABC, C00, C0, OMEG1, P, R1, R2, TM, XNRHO
REAL NU, NUS, NU0, NU1, NU2, NU3, NU4, NU5
PI=3.14159
FIS=PI*PI
NU=C/1.315246E-4
NUS=NU*NU
FISNUS=FIS*NUS*4.
G=0
CS=C*C
NU0=NU
NU1=NU0+.141*C
NU2=NU1+.068*C
NU3=NU0-.427*C
NU4=NU3-.026*C
NU5=NU4-.068*C
DELTA23=NU-NU5
DELTA22=NU-NU4
DELTA21=NU-NU3
DELTA34=NU-NU0
DELTA33=NU-NU1
DELTA32=NU-NU2
TEMPO=293
TWALL=TEMPO
T1=TWALL
A=5.434
A1=A*2.4/7.7*CS
A2=A*3.0/7.7*CS
A3=A*2.3/7.7*CS
A4=A*5.0/7.7*CS
A5=A*2.2/7.7*CS
A6=A*0.6/7.7*CS
FUGTEMP=SQRT(T1/300.)
ALPHAM=1.88E7*FUGTEMP
DELDOF=2.51E8*FUGTEMP
DELNU=DELDOF+ALPHAM*P
SIGMA23=A1/(FISNUS*DELNU)/(1+(2.*DELTA23/DELNU)**2)*5./12.
SIGMA22=A2/(FISNUS*DELNU)/(1+(2.*DELTA22/DELNU)**2)*5./12.
SIGMA21=A3/(FISNUS*DELNU)/(1+(2.*DELTA21/DELNU)**2)*5./12.

```



```

SIGMA34=A4/(FISNUS*DELNU)/(1+(2.*DELTA34/DELNU)**2)*7./12.
SIGMA33=A5/(FISNUS*DELNU)/(1+(2.*DELTA33/DELNU)**2)*7./12.
SIGMA32=A6/(FISNUS*DELNU)/(1+(2.*DELTA32/DELNU)**2)*7./12.
SIGMAT=SIGMA23+SIGMA22+SIGMA21+SIGMA34+SIGMA33+SIGMA32
SIG=SIGMAT
RETURN
END

```

```

SUBROUTINE INTEG(IPRINT,H)

```

```

  THIS SUBROUTINE INTEGRATES THE SYSTEM OF DIFFERENTIAL EQUATIONS
  DEFINING THE CHEMICAL KINETICS OF N-C3F7I IODINE LASER

```

```

  USING A VARIABLE STEP SIZE 7TH ORDER RUNGE KUTTA-FEHLBERG METHOD.

```

```

  IMPLICIT REAL*8(A-H,K,L,O-Z)

```

```

  DIMENSION YD(7),X(7),WK(84)

```

```

  COMMON/BLK1/X7,POWER

```

```

  COMMON/BLK3/B,B2,B3,C,A00,B00,EFSNU,OMEGA,C6

```

```

  COMMON/BLK4/CHSI10,CHSI20,ABARO,Z1BAR,LC,XK0

```

```

  COMMON/BLK7/ABC,C00,C0,OMEG1,P,R1,R2,TM,XNRHO

```

```

  COMMON/BLK8/ZOL,ZE,NG,TO,RAD,A,PIN,W

```

```

  COMMON/BLK22/AD,V1,V2,GG

```

```

  COMMON/BLK23/W0,ETA0,PT0,FRAC

```

```

  COMMON/BLK29/ZZZ,TZZ,PZZ,ETAZZ,WZZ

```

```

  COMMON/BLK30/DATA(50,50),NDMAX,FLRATE(8),FDPTDAT(50,40)

```

```

  EXTERNAL FUN,CHSI1,CHSI2

```

```

  REAL LC

```

```

  INTEGRATE SYSTEM FROM S=0 TO S=1.0 USING RUNGE-KUTTA METHOD

```

```

  X(1)=RI

```

```

  X(2)=R

```

```

  X(3)=R2

```

```

  X(4)=I2

```

```

  X(5)=I*

```

```

  X(6)=I

```

```

  X(7)=RHO+

```

```

  X8=RHO-

```

```

  X9=I*-.5*I

```

```

  INITIALIZE CONSTANTS FOR FLOW EQUATIONS

```

```

  SEE COMMON BLK10 FOR THESE CONSTANTS--NEEDED FOR SUB FLOW

```

```

  CALL PFLOW

```

```

  ND=0

```

```

  TEST FOR PRINT CONDITIONS

```

```

  IF(IPRINT.EQ. 0) GO TO 229

```

```

  NG=NG+1

```

```

  NG IS THE NUMBER OF GRAPHS TO BE SAVED

```

```

  MAXIMUM NG=8

```

```

  FLOWRATE(NG) IS LABEL FOR DATA SAVED

```

```

  SEE ALSO PROGRAM PLOTD--WHICH CAN PLOT THE SAVED DATA

```

```

  FLRATE(NG)=OMEGA

```

```

  WRITE(8,331) LC

```

```

331     FORMAT(1X,11H   LC   =  ,F10.2)
229     CONTINUE
55      CONTINUE
      N=7
      TOL=1.0E-5
      PD=1.0
      MTH=1
      WZZ=W0
C      H IS STEP SIZE IN SCALED UNITS BETWEEN PRINT OUTS
C      IPRINT=0 OFF, IPRINT=1 ON
      HMIN=1.0E-9
      HMAX=H/100.
      HUSE=HMIN*1000.
      IERR=0
C      INITIAL CONDITIONS
      Z0=0.0
      Y0(1)=1.0
      Z1=0.0
      DO 9 I=2,6
9       Y0(I)=0.0
C      INITIALIZE FLOW,DENSITY,PRESSURE AND TEMPERATURE AT Z=0
      CALL FLOW(Z0,TEMP,PRESS,FLWR,DENSITY,DWDZ)
C      GUESS AT INITIAL CONDITIONS FOR X(8)
      X70=PIN*W/(EPSNU*C)
C      X70 IS RHO+(0) WHICH IS GIVEN
C      INITIAL CONDITION FOR RHO-(0) IS UNKNOWN--ASSUME C00 VALUE
      XK0=X70*C00
      X8=XK0/X70
      Y0(7)=X70/B
      IF(IPRINT.EQ. 0) GO TO 300
      CALL FUN(N,Z0,Y0,F)
      TEMP=TZZ+273.
      IF(Z0.EQ.0.0)CALL PRINT(Z0,TEMP)
      WRITE(6,191)
191     FORMAT(///,T7,1HZ,T20,4H[R1],T32,4H[R1],T45,5H[R2],T57,4H[I2],
1       T69,4H[I*],T80,4H[I] ,T91,6H[RHO+],T103,6H[RHO-],T112,
2       9HINVERSION      )
300     CONTINUE
      DO 10 I=1,7
10      X(I)=B*Y0(I)
C
      X8=XK0/X(7)
      X9=X(5)-.5*X(6)
      X7STAR=X(7)+X8
C      USE SUBROUTINE SIGMA TO CALCULATE CROSS SECTION SIGMA
      CALL SIGMA(SIG2)
      IF(IPRINT.EQ. 0) GO TO 222
      WRITE(6,199)Z0,(X(I),I=1,7),X8,X9
      WRITE(6,303)ZZZ,TZZ,PZZ,ETAZZ,WZZ
      CALL FUN(N,Z0,Y0,F)
      TEMP=TZZ+273.
      IF(Z0.EQ.1.0)CALL PRINT(Z0,TEMP)
222     CONTINUE
C      SAVE THE DATA FOR FUTURE PLOT ROUTINES
C      DATA ARRAYS ARE DATA(50,50) AND FDPTDAT(50,40)
C

```

```

      IF(IPRINT .EQ. 0) GO TO 227
      ICOL=(NG-1)*6
      ND=ND+1
      DATA(ND,ICOL+2)=X(2)
      DATA(ND,ICOL+1)=Z0
      DATA(ND,ICOL+3)=X(4)
      DATA(ND,ICOL+4)=X(5)
      DATA(ND,ICOL+5)=X(6)
      DATA(ND,ICOL+6)=X9
      NNN=(NG-1)*5
      FDPTDAT(ND,NNN+1)=Z0
      FDPTDAT(ND,NNN+2)=WZZ
      FDPTDAT(ND,NNN+3)=ETAZZ
      FDPTDAT(ND,NNN+4)=PZZ
      FDPTDAT(ND,NNN+5)=TZZ
C      WRITE(Z,R,I2,I*,I,INV
      WRITE(8,6773) Z0,X(2),X(4),X(5),X(6),X9
      WRITE(8,6773) Z0,WZZ,ETAZZ,PZZ,TZZ
6773  FORMAT(1X,F6.3,2X,5(2X,E15.6))
227  CONTINUE
      IF(Z0.LE.0.0) GO TO 3567
      IF(IPRINT .EQ. 0) GO TO 223
      WRITE(6,303) ZZZ,TZZ,PZZ,ETAZZ,WZZ
223  CONTINUE
303  FORMAT(1X,T2,3HZ= ,F10.3,2X,T15,3HT= ,F7.3,2X,T30,
1 7HPTORR= ,F9.4,2X,
2 T55,9HDENSITY = ,F9.6,2X,T80,3HW= ,E14.7 )
3567 CONTINUE
199  FORMAT(1X,E12.5,8E12.5,E12.5 ,E12.5 )
C
C
C      USE 7TH ORDER RUNGE KUTTA INTEGRATION SCHEME WITH VARIABLE STEP
C      STEP SIZE CAN VARY FROM HMIN TO HMAX
C      Z0 IS STARTING VALUE FOR Z
C      Z1 IS NEXT STOPPING POINT IN INTEGRATION SCHEME
C      TOL IS TOLERANCE
C      IERR IS ERROR CODE TO DETERMINE IF INTEGRATION WAS SUCCESSFUL
C
100  CONTINUE
      Z1=Z1+H
      IF(Z1 .GT. 1.00) GO TO 111
      CALL RK7(N,Z0,Z1,Y0,TOL,FUN,PD,MTH,HMIN,HMAX,HUSE,WK,IERR)
      IF(IERR .NE. 0) WRITE(6,444) IERR,Z0,Z1,(Y0(I),I=1,7)
      IF(IERR .NE. 0) STOP 1717
444  FORMAT(1X,18HIERR IS NOT ZERO ,I5, (4E16.7,/))
200  CONTINUE
      X(7)=B*Y0(7)
      XB=XK0/X(7)
60  FORMAT(1X,5(2X,E14.6))
      GO TO 300
500  CONTINUE
      DO 110 I=1,7
110  X(I)=B*Y0(I)
      XB=XK0/X(7)
      X9=X(5)-.5*X(6)

```

```

111      CONTINUE
        XX7L=X(7)
C      X(7) IS CALCULATED RHO+(L) VALUE
        XKCAL=R2*X(7)*X(7)
C      XKCAL IS CALCULATED VALUE FOR XK0
C      ABC IS DIFFERENCE BETWEEN CALCULATED AND INITIAL VALUE
        DIF=((XK0-XKCAL)/XKCAL)*100.
        ABC=DIF
        IF(IPRINT .EQ. 0) GO TO 224
        WRITE(6,202)DIF,XKCAL,XK0,C00
224      CONTINUE
202      FORMAT(1X,13HDIFFERENCE = ,E18.9,2X,12HXKCAL    =    ,E18.9,
1 2X,10HXK0    =    ,E18.9,2X,6HC00 =    ,E18.9 )
237      CONTINUE
C
C      RHOMIN=RHO-(0)=XK0/RHO+(0)=XK0/X70
        RHOMIN=XK0/X70
        FOUT=RHOMIN*W*EPSNU*C
        GAINDB=10.*ALOG10(FOUT/PIN)
        GAIN=FOUT/PIN
        IF(IPRINT .EQ. 0) GO TO 226
        WRITE(6,193)R1,R2,P,PIN,FOUT,GAINDB,GAIN
226      CONTINUE
193      FORMAT(1X,5HR1 = ,F10.7,2X,5HR2 = ,F10.7,1X,
1 6HPRESS = ,F10.7,2X,6HPIN = ,E14.7,3X,7HPOUT = ,E14.7,/,
2 1X,9HGAINDB = ,E14.7,3X,7HGAIN = ,E14.7 )
501      CONTINUE
        NDMAX=ND
C      NDMAX IS THE MAXIMUM NUMBER OF DATA POINTS
        RETURN
        END

```

**APPENDIX B**

**OUTPUT FROM SIMULATION MODEL**

# INPUT PARAMETERS

PTO - 15.0  
 OMEG1 - 3000  
 CON - 1689  
 COO - 2,13398E8  
 R1 - 0.00  
 R2 - 0.9584792  
 LC - 1000  
 ZOL - 500  
 XNRHO - 1.0  
 TO - 300.0

## OUTPUT

<u>P<sub>in</sub></u>	<u>P<sub>out</sub></u>	<u>Gain</u>	<u>Gain db</u>
10.0	128.4570	12.8457	11.0875
5.0	124.9000	24.9801	13.97595
2.0	122.2330	61.1166	17.8616
1.0	119.9611	119.9611	20.7904
0.5	116.9325	233.8649	23.6895
0.2	111.3596	556.798	27.4570
0.1	105.7950	1057.954	30.2446
0.01	80.3968	8039.678	39.0524

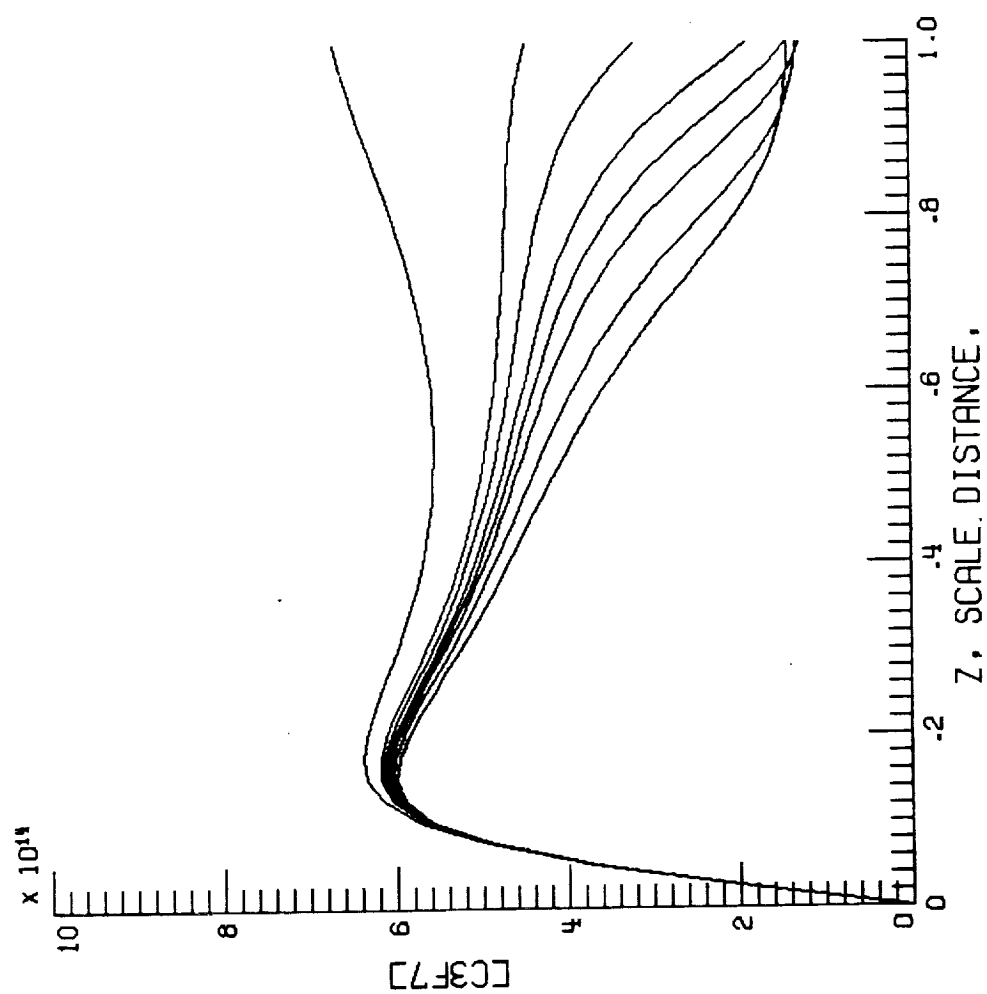


Figure 1.

INFOPLT 1

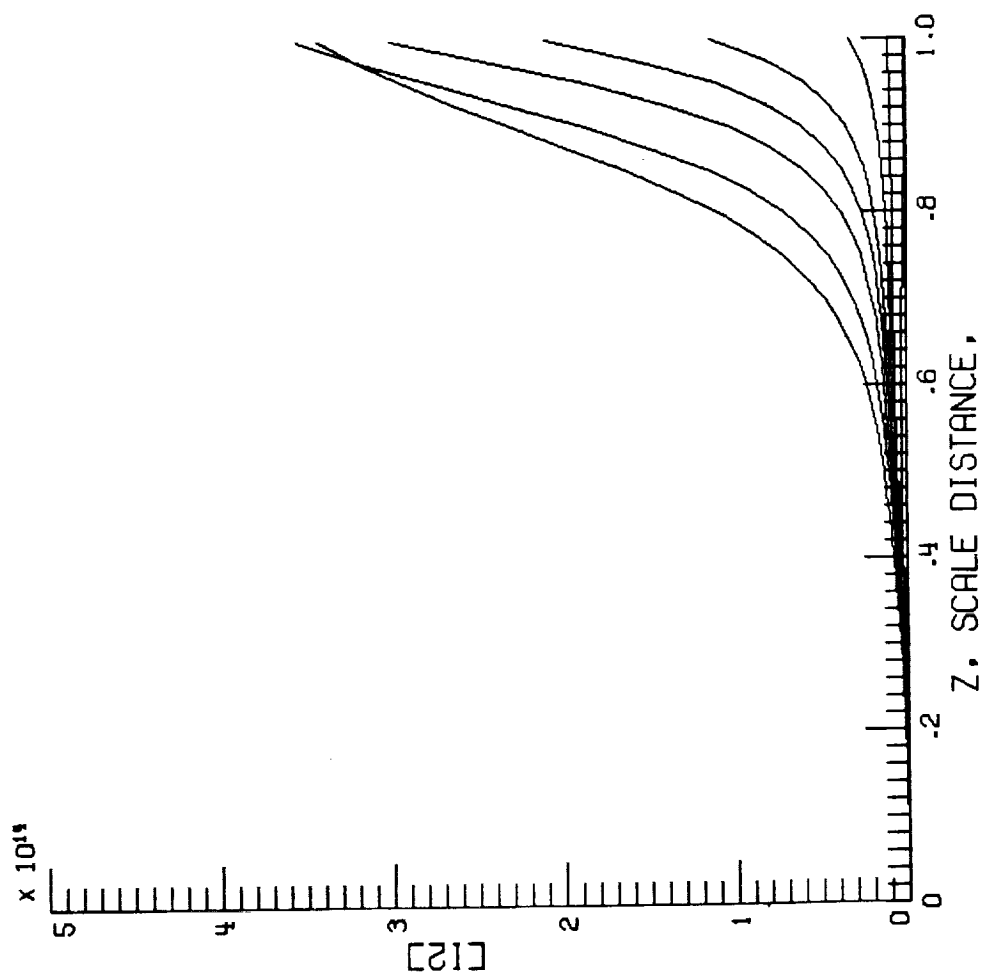
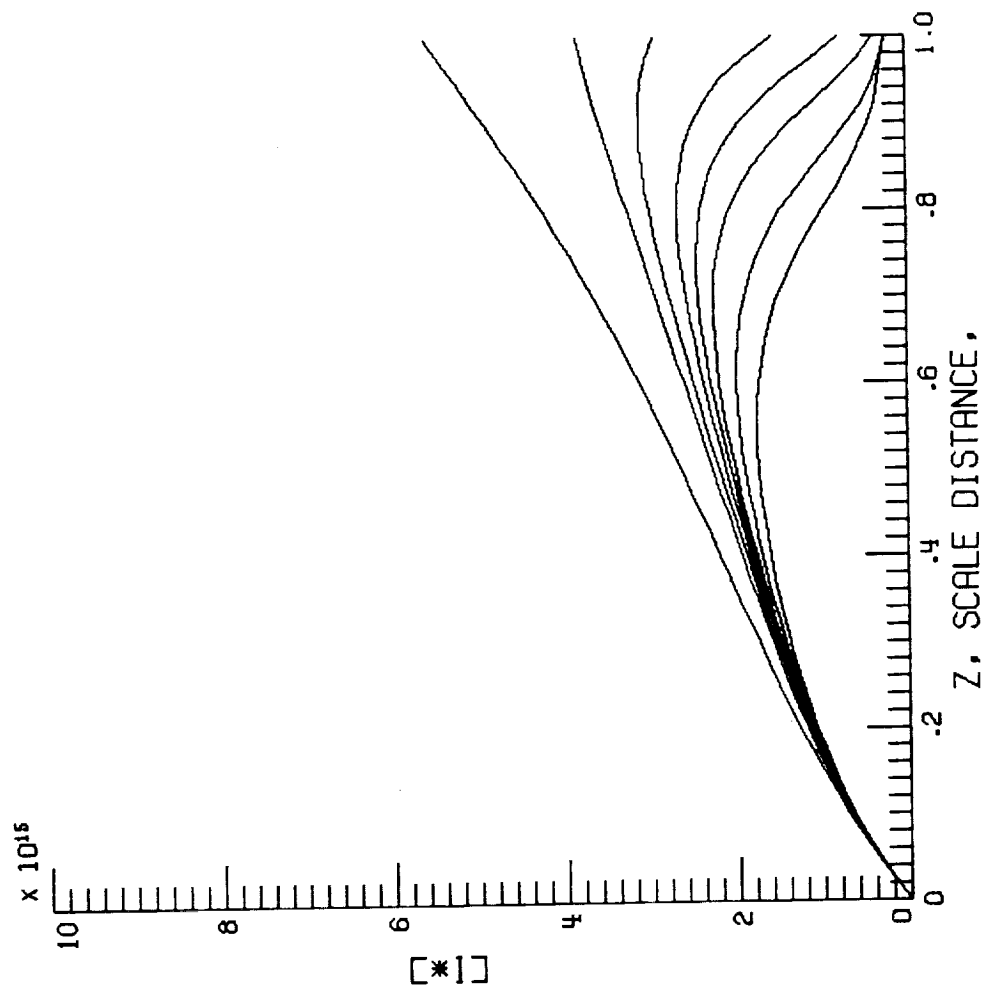


Figure 2.

INFOPLT 2.





INFOPLT 3.

Figure 3.

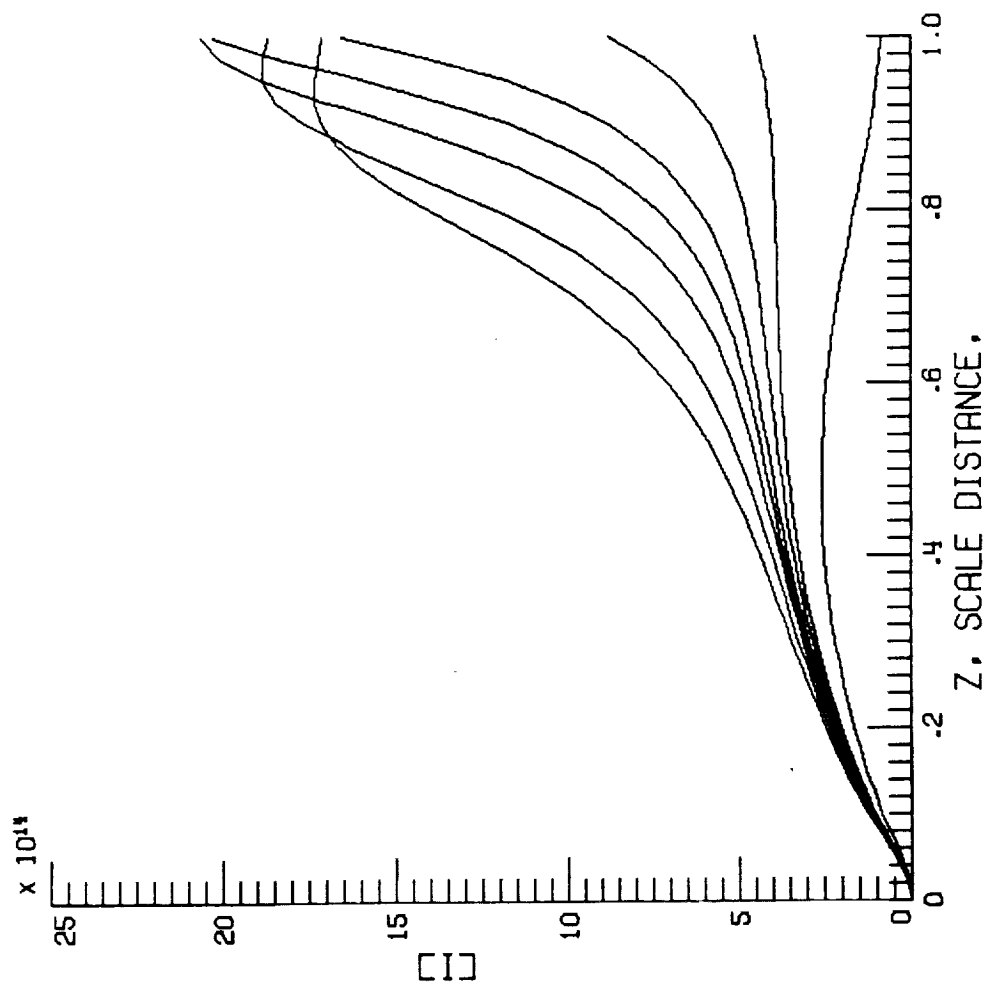


Figure 4.

INFOPLT 4.

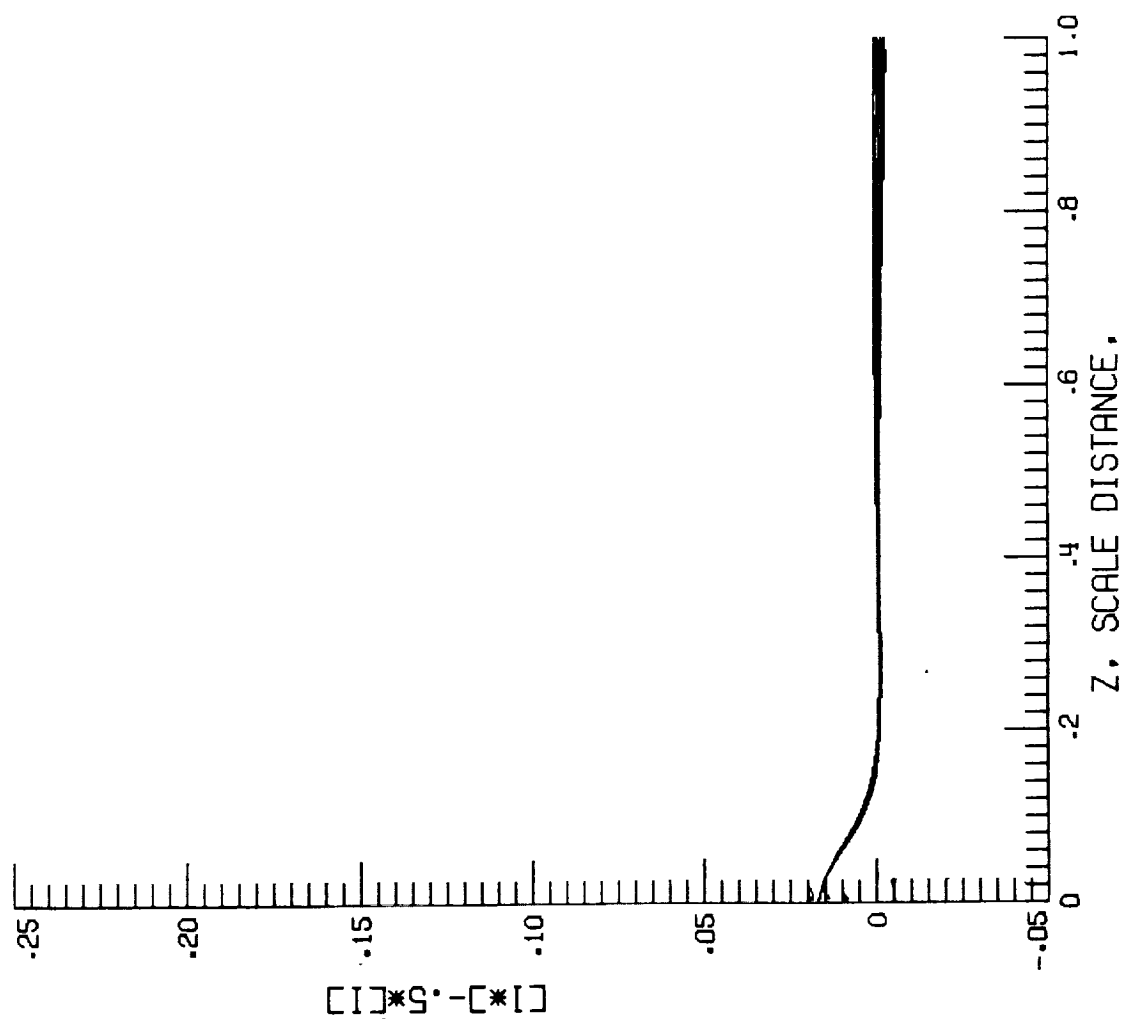


Figure 5.

INFOPLT 5.

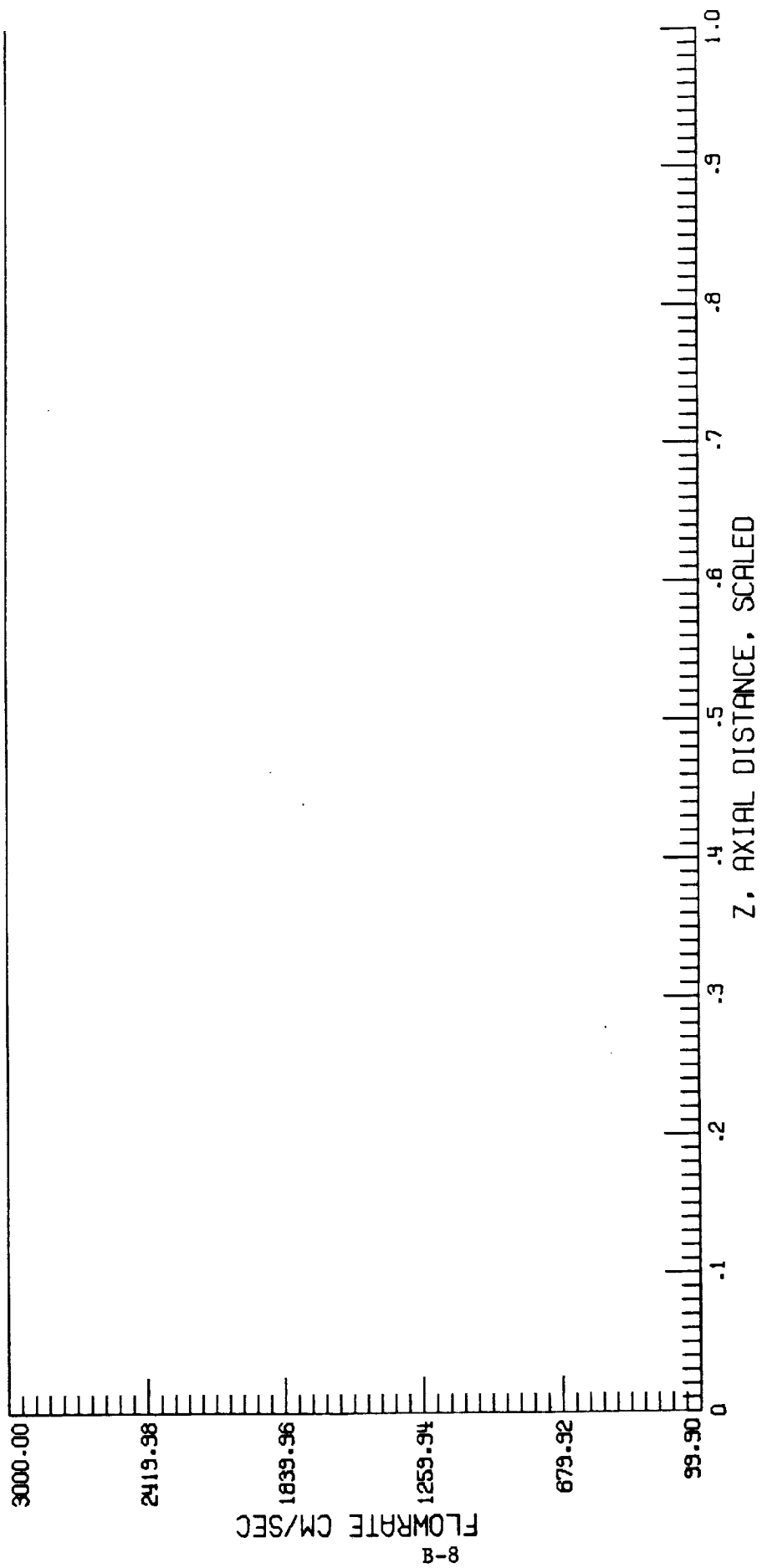


Figure 6.

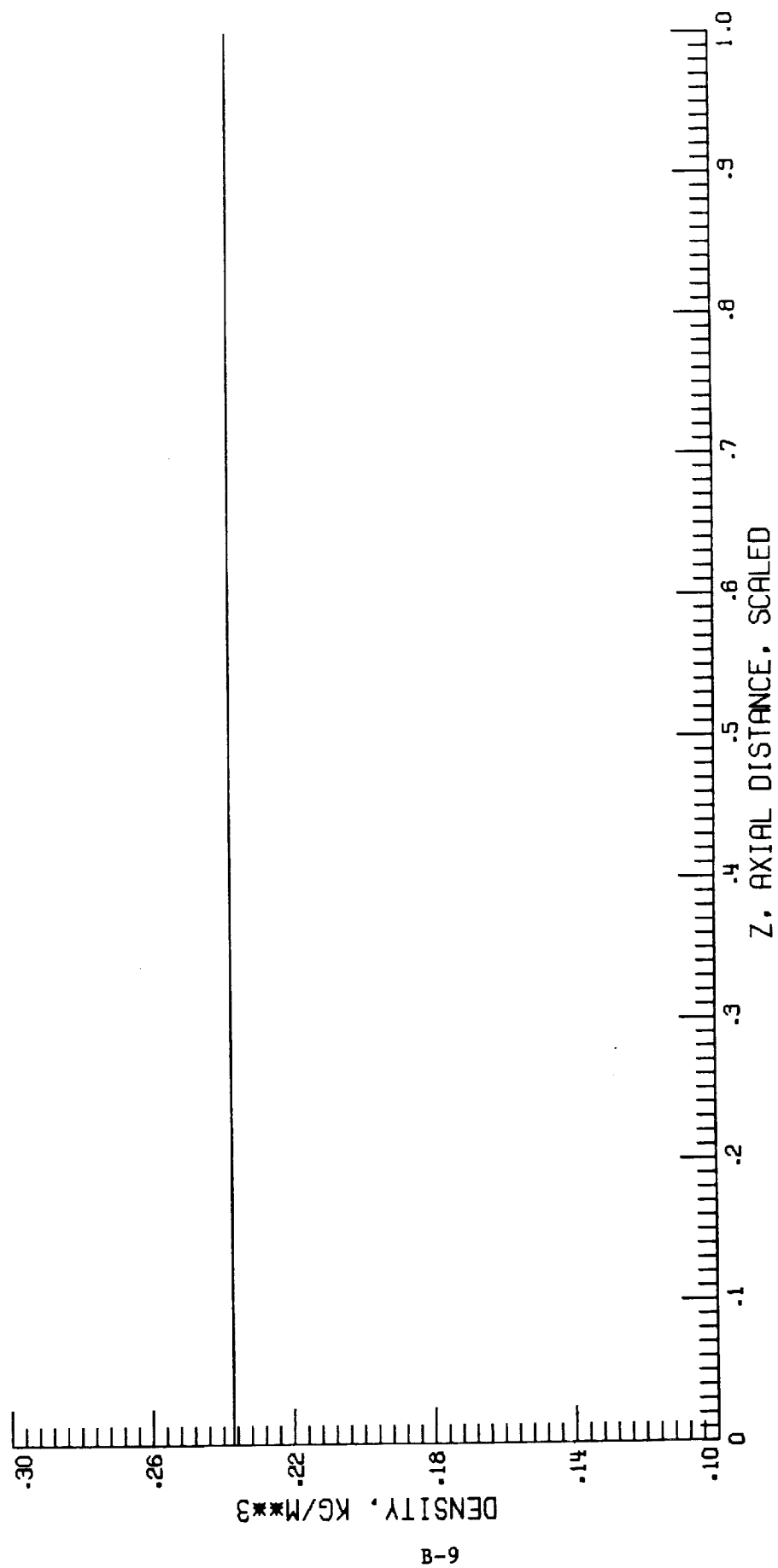


Figure 7.

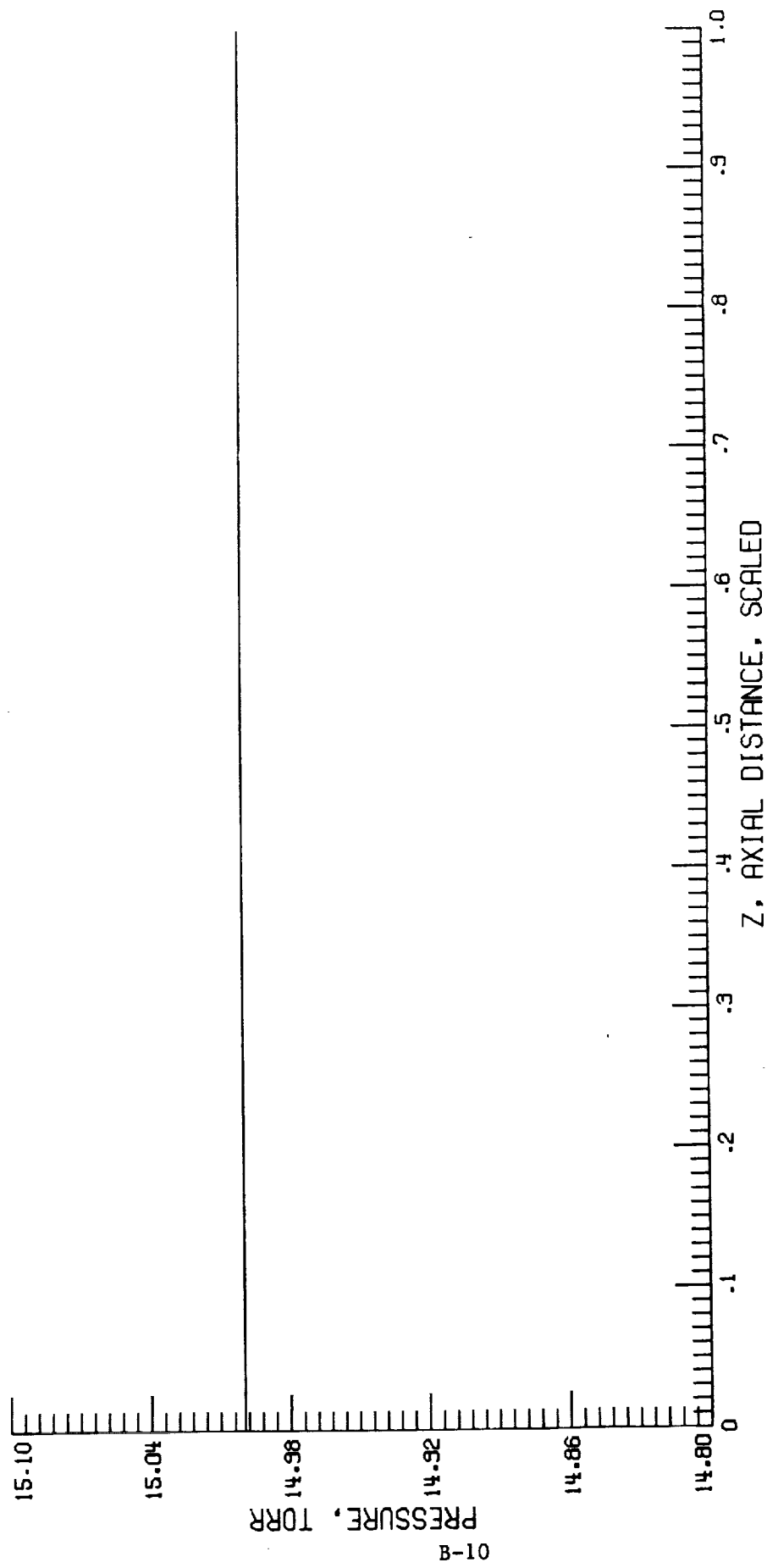


Figure 8.

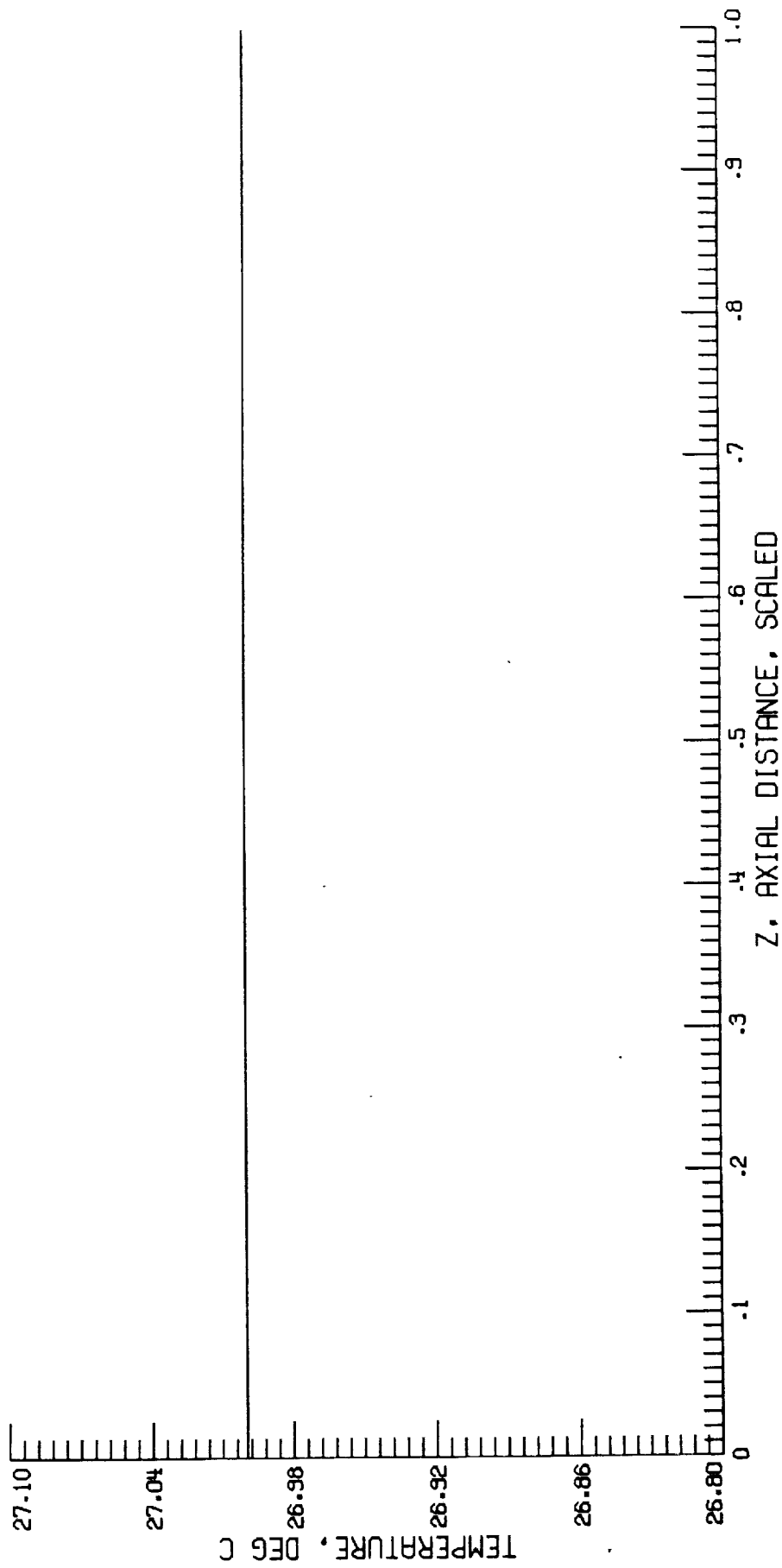


Figure 9.